Surfactant-Based Chemical and Biological Agent Decontaminating Solution Development

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Background

- **Current Decontaminating (Decon) Solutions (Navy HTH and Army DS-2) Are:**
  - **Toxic**
  - **Corrosive to Materials**
  - **Environmentally Unfriendly**
- **Joint Service Family of Decon Systems (JSFDS) Program Requirement for New Decon**
  - **Must Be As Effective As Current Decons**
  - **Effective Against Biological Agents**
  - **Compatible (Noncorrosive) with Military Materials**
  - **Environmentally "Green" and Nontoxic to User**

Objectives

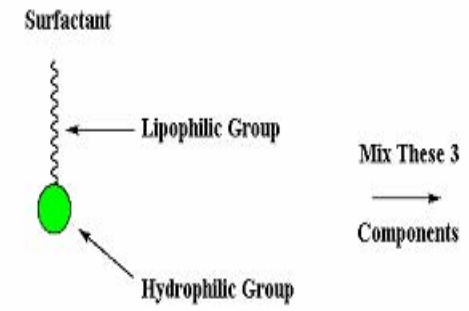
- **Develop a Surfactant-Based Decon Solution That Will Meet JSFDS Requirements**
- **Most Challenging Requirements**
  - **Neutralization Time of 15 Minutes for VX, HD, and TGD**
  - **Pot Life of 12 Hours**
  - **Disinfect Vegetative and Endospore Forming Bacteria, Fungi, and Viruses in 15 Minutes**
  - **Noncorrosive to Military Materials**
  - **Nontoxic and Environmentally "Green"**

Decon Formulation Components

- **Surfactants**
  - Use to Replace Organic/Halogenated Solvents to Solubilize Chemical Agents
  - Must Be Stable Against Oxidation and Hydrolysis
  - Utilize to Increase Biocidal Efficacy by Lowering Interfacial Tension Between Spores and Biocide
- **Peroxygen Compound**
  - Utilize as Environmentally Green Reactant for Both Chemical and Biological Agents
  - Some Peracids Available in Neat Form (Peracetic acid) and In-Situ (Commercial Detergent Technology)
- **Catalyst**
  - Promote Oxidation of the Sulfur in V and HD
  - Reported to Promote Hydrolysis at Lower pH (for G Agent Decontamination)

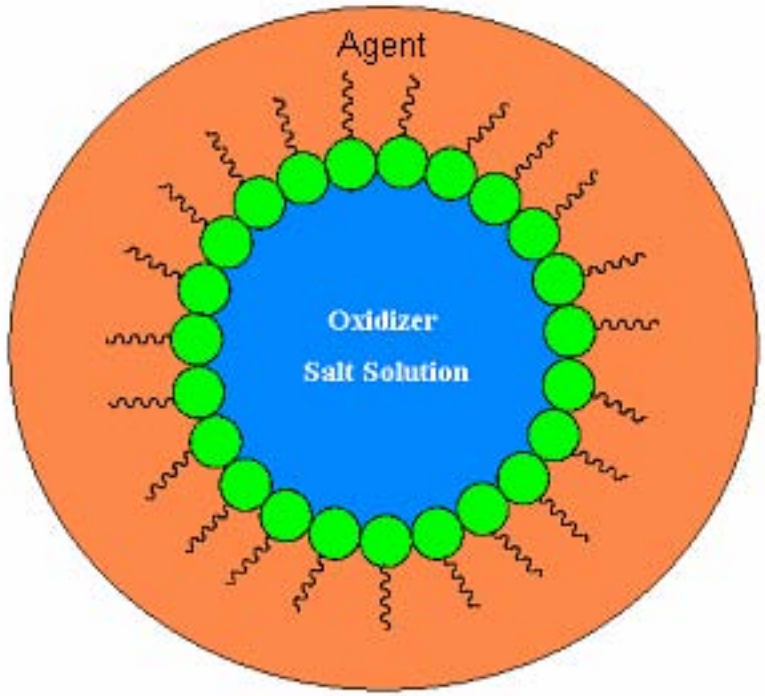
Decon Formulation Components - Surfactants

- **Basics of Microemulsion Formulation**



Mix These 3 → Components

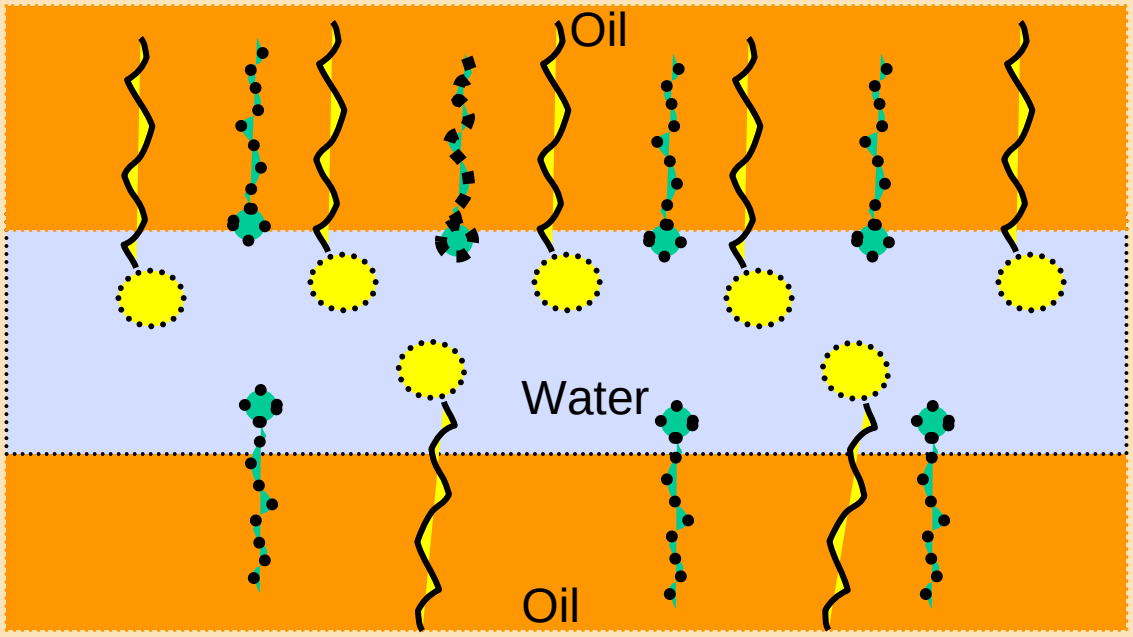
Agent - Nonpolar Molecules (Liquid)
Oxidizer - Polar Molecules (Liquid)



Water-in-Oil Microemulsion

Decon Formulation Components - Surfactants

- **MICROEMULSION FORMULATION**
  - **Identify surfactant(s) slightly soluble in the aqueous phase**
  - **Identify surfactant(s) slightly soluble in the oil phase**
  - **Combine oil soluble and water soluble surfactants to reduce interfacial tension between oil and water phase to produce microemulsion**



Decon Formulation Components - Surfactants

- **Surfactant / Solubility Screen**

J A B C D E F G H I

Oil/Water = 20/80; Surfactant = 3%; Oil = Dibutylsulfide; Water = water + 500-mg Na carbonate

J: control
A: C_{16} Diphenyloxide sulfonate
B: C_{14-17} sec-Alkyl sulfonate
C: C_{6-16} Cocamidopropylamine oxide
D: C_{10} Amine oxide
E: C_{12} Amine oxide
F: C_{14} Amine oxide
G: C_{12-18} Amine oxide
H: C_{18} Amine oxide
I: di-C_{10} Amine oxide

Decon Formulation Components - Surfactants

- **Surfactant Scan – Amine Oxides**

	J	A	B	C	D	E	F	G
S1/S2=		100/0	90/10	75/25	50/50	25/75	10/90	0/100

O/W = 20/80; (S1+S2) = 3%; V(T) = 5-mL; O = Dibutyl sulfide, W = water + 500-mg Na carbonate

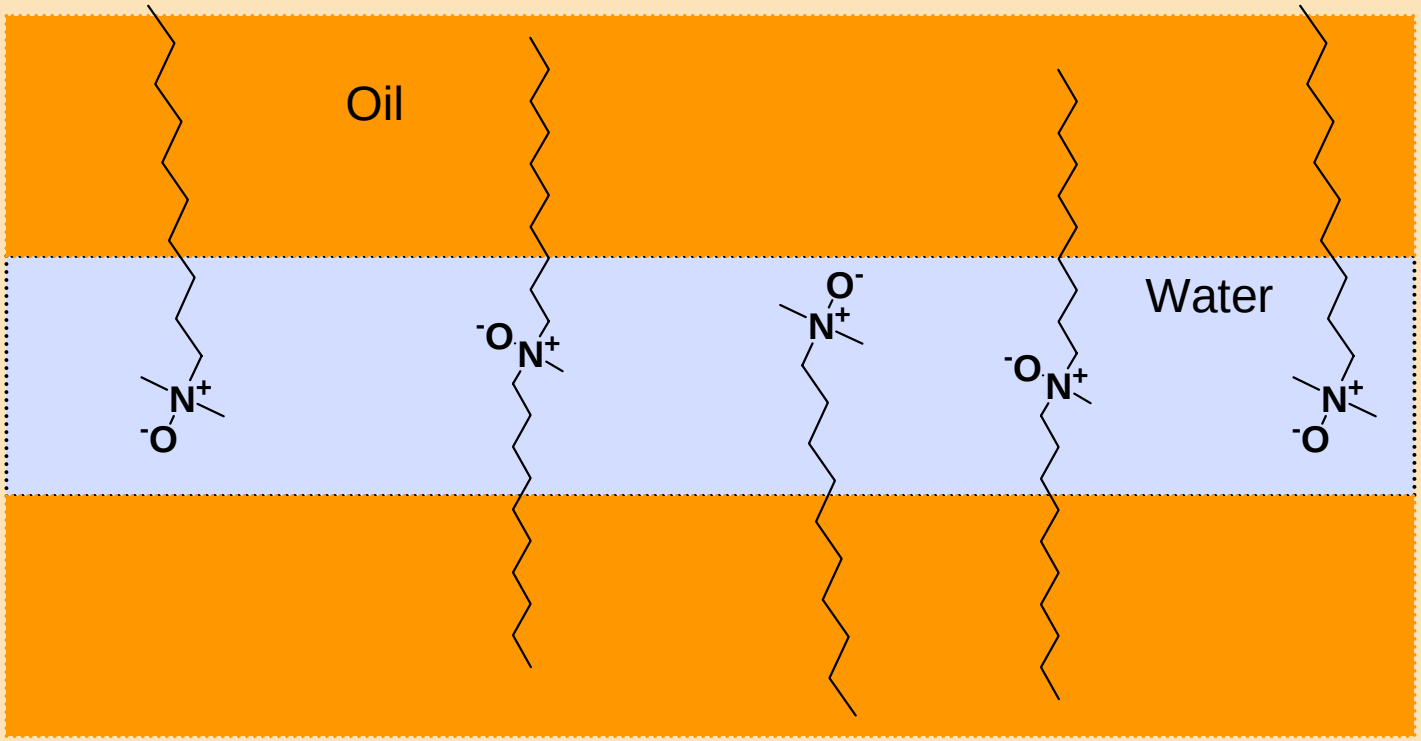
J: control (no surfactant),

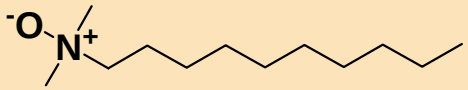
S1: C_{10} Amine oxide

S2: di-C_{10} Amine oxide

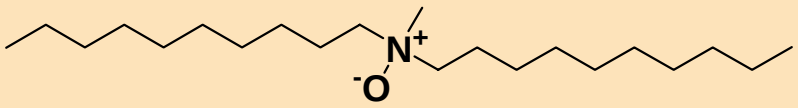
Decon Formulation Components - Surfactants

- **Current System - Mixed Amine Oxide Surfactant Microemulsion**





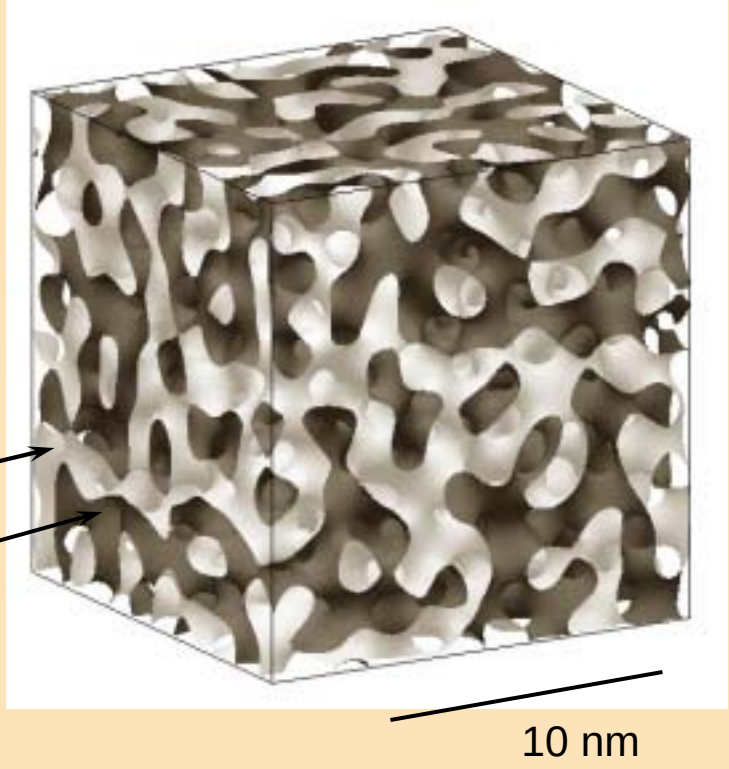
C_{10} Amine oxide. Dimethyldecylamine oxide



Di-C_{10} Amine oxide. Didecylmethylamine oxide

Decon Formulation Components - Surfactants

- **Why Microemulsion?**
  - **Increased Stability**
  - **Increased Reactivity (Surface Area)**



Decon Formulation Components – Peroxygen Compound

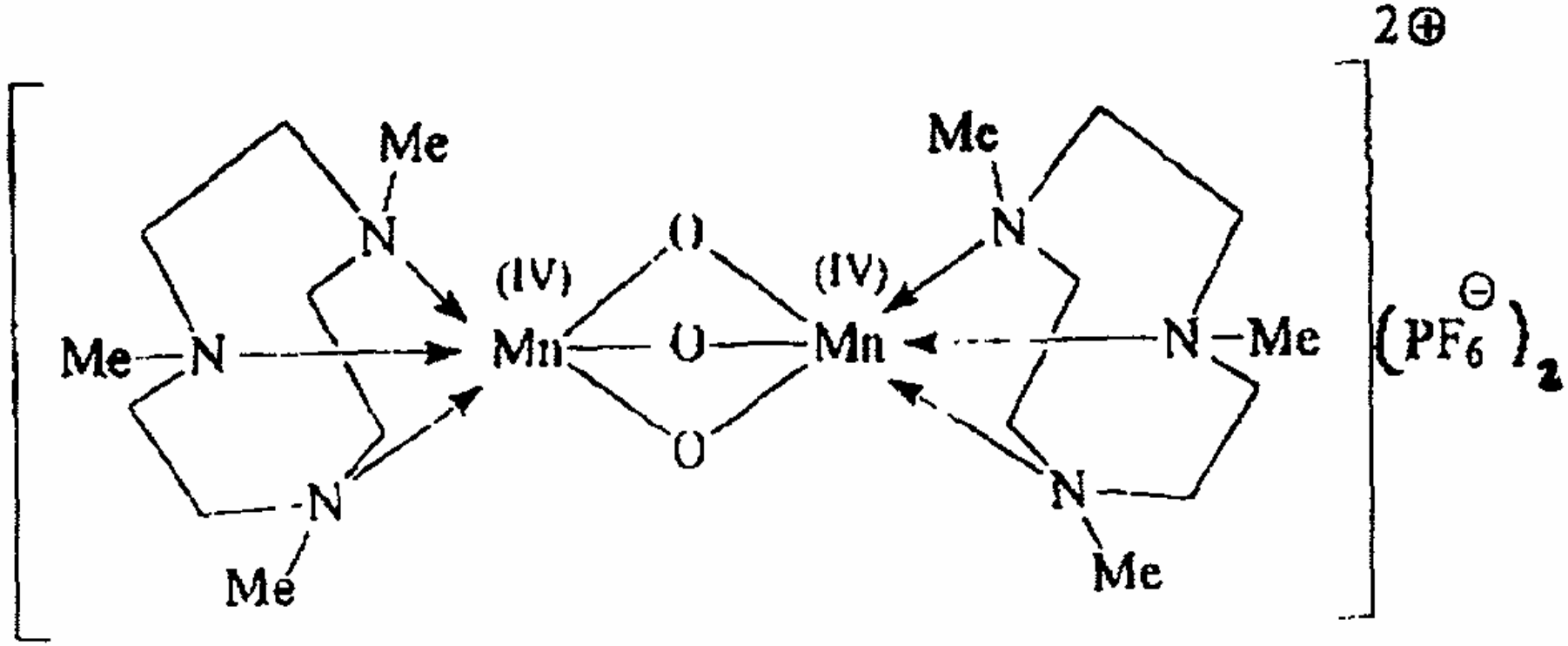
- **Peroxgen Compounds**
  - **Organic Peroxides (t-Butyl hydroperoxide)**
    - Requires Catalyst to Meet Decon Reactivity Requirement
    - Stable - Does Not Require Special Handling
    - One of Two Organic Peroxides That Meet DOT Shipping Regs for Bulk Shipment
  - **Peracids**
    - Strong Oxidizers
    - Broad Spectrum Disinfectants
    - Use Neat or Generate In-Situ (Tide With Bleach)
    - Stability (Handling / Storage) Can Be an Issue

Decon Formulation Components – Catalyst

- **Dimanganese-Based Complex**
  - **Developed for Laundry and Detergent Industry**
  - **Catalyst Activates Stain (** $Mn^{4+} + e^{-} \rightarrow Mn^{+3}$ **)**
  - **Stain More Susceptible to Bleach (Oxidation)**
- **Macrocylic Tetradentate Liqand (TAML)**
  - **Developed by Carnegie Mellon**
  - **Complexes the Peroxygen**
  - **Stable in Presence of Strong Oxidants**
  - **Defluoro Reported to Promote Hydrolysis and Oxidation at Lower pH**

Decon Formulation Components – Catalyst

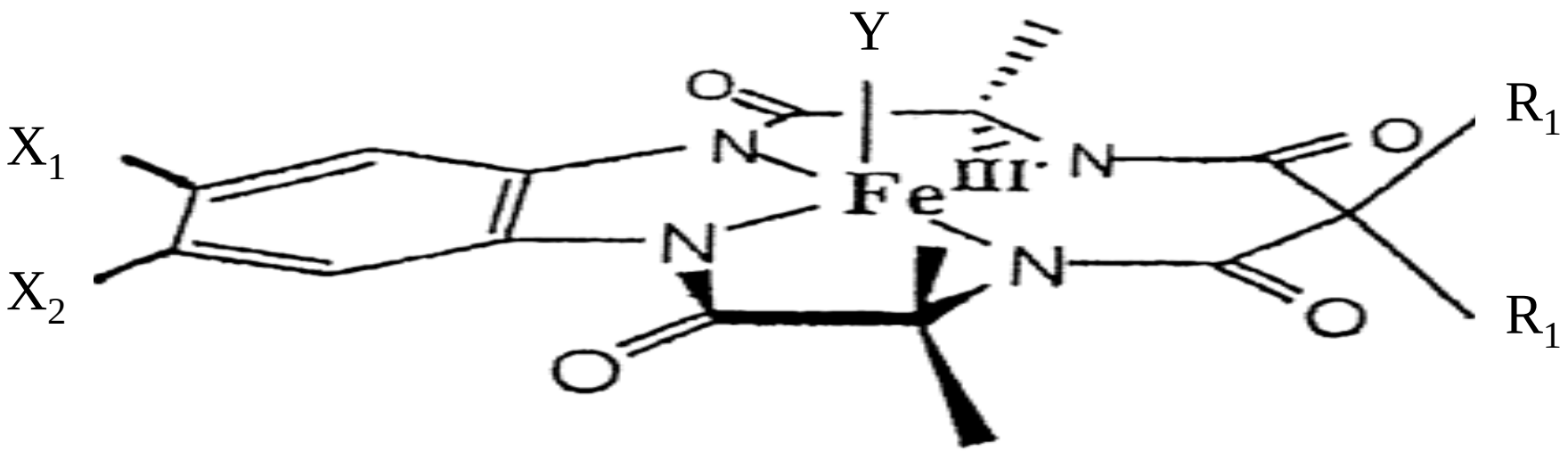
- **Dimanganese-Based Complex**
  - **1,4,7-Trimethyl-1,4,7-trizacyclononane ligands (Me3TACN)**



Decon Formulation Components – Catalyst

- **Macrocylic Tetradentate Ligand**

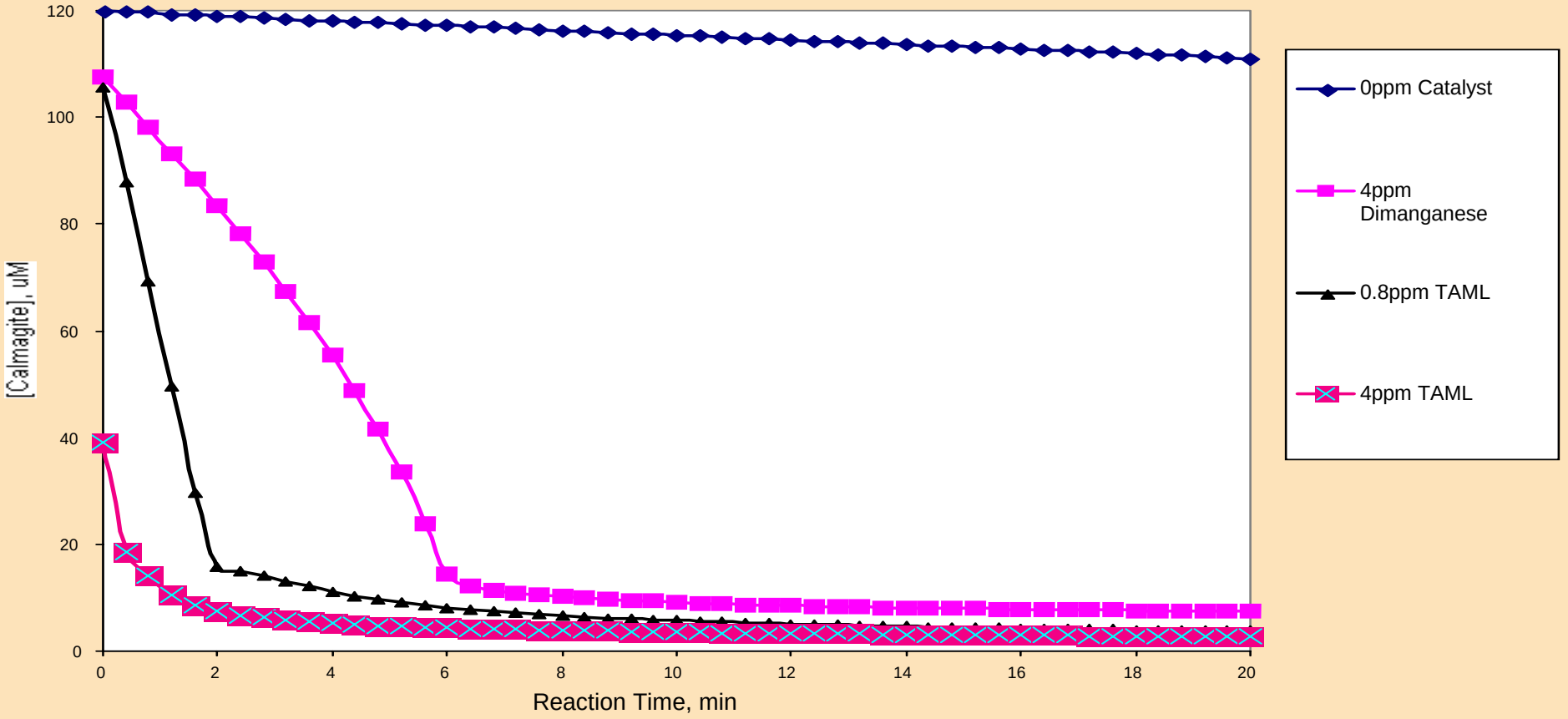
	X_1	X_2	R_1
– FeMB	Me	H	Me
– FeB	H	H	Me
– FeF_2B	H	H	F
– FeF_2DCB	Cl	Cl	F



Decon Formulation Components – Peroxygen Compound and Catalyst

Oxidation of Calmagite Dye by t-Bu Hydroperoxide

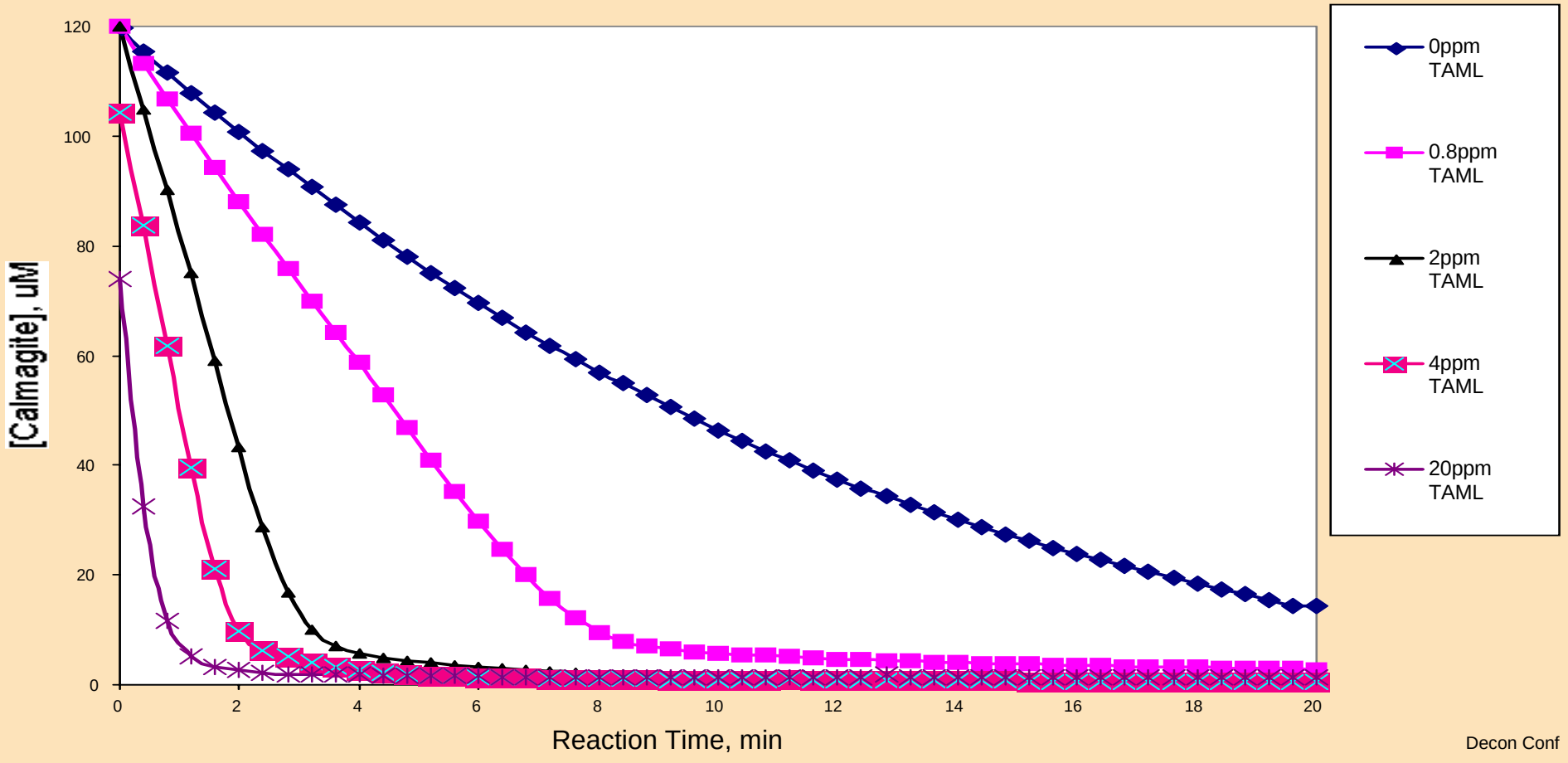
TAML FeMB and Dimanganese Catalysts



Decon Formulation Components – Peroxygen Compounds and Catalysts

Oxidation of Calmagite Dye by Peracetic Acid

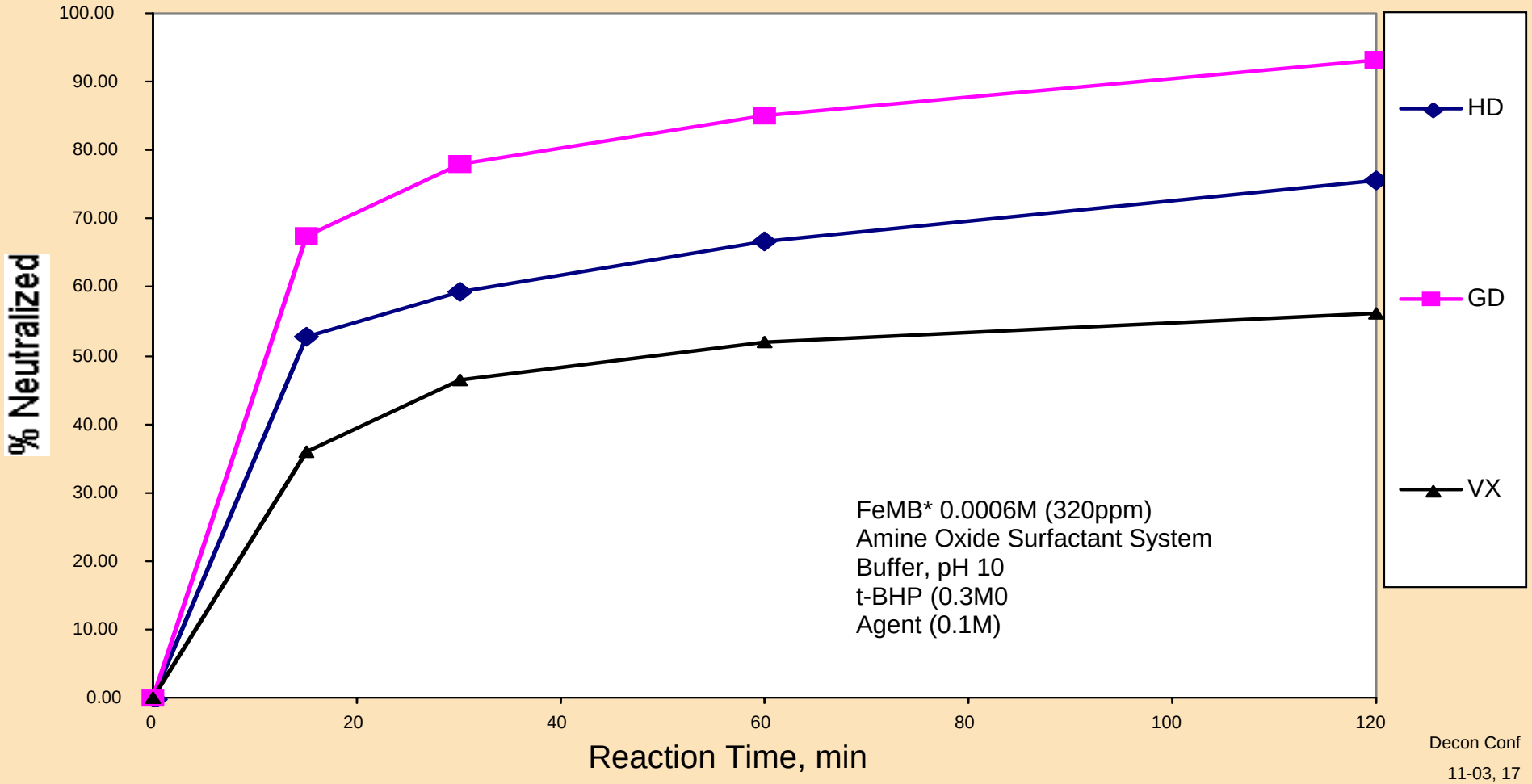
TAML FeMB Catalyst



Decon Formulation Components – Peroxygen Compounds and Catalysts

Agent Decontamination by t-Bu Hydroperoxide in Microemulsion

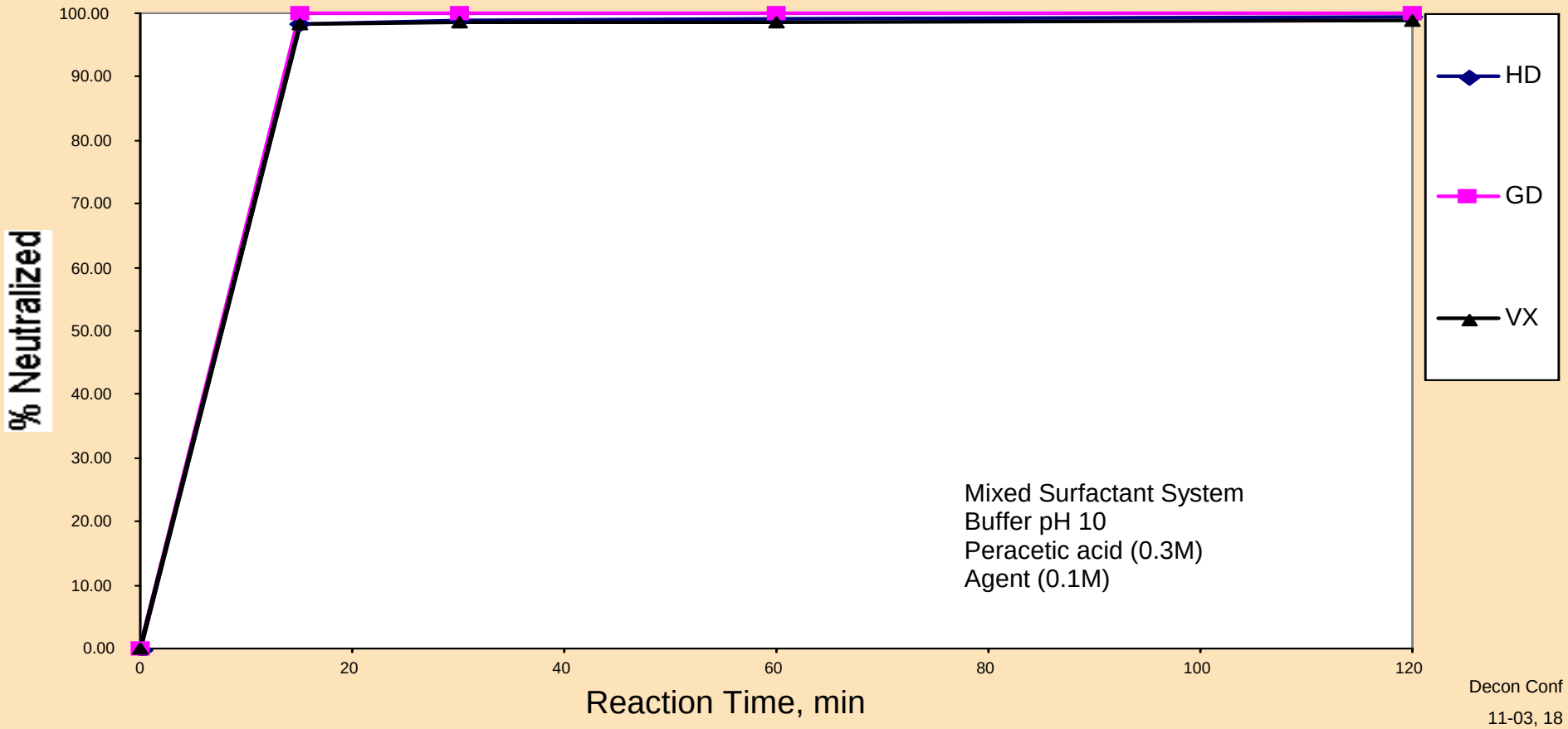
TAML FeMB Catalyst



Decon Formulation Components – Peroxygen Compounds and Catalysts

Agent Decontamination by Peracetic Acid

Uncatalyzed



Biological Decontamination

- **Peracetic Acid (PAA) Found to Be an Effective Disinfectant**

Reduction in *Bacillus globigii* after 15 minute Exposure to Candidate Solutions

	BG Initial CFU/mL	Log Reduction, CFU/mL
Damox 1010 (1)	**10^6**	**0 (30 min exposure)**
Barlox 10S (2)	**10^6**	**0 (30 min exposure)**
PAA, 5%	**10^8**	**4**
PAA in uEm	**10^8**	**8**

(1) C_{10} Amine oxide

(2) di-C_{10} Amine oxide

Summary

- **Microemulsions Developed From Oxidation and Hydrolysis Resistance Surfactants**
- **Peracids (Peracetic) Demonstrated Efficacy Against Chemical Agents (HD, VX, GD)**
  - **Efficacy Achieved Without Catalyst**
- **Peracids (Peacetic) Demonstrated Efficacy Against Biological Agent Simulant (BG)**